STUDIES OF THE SUBSTITUTION EFFECTS ON THE ELECTRONIC PROPERTIES FOR BIPHENYL AND DERIVATIVE MOLECULES BY USING DFT METHOD

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Abstract. DFT method has been carried out to study the substitution effects of NO_2 group on the electronic properties (ionization potential, electron affinity, electronegativity, hardness, softness and electrophilicity index) and IR spectral properties of biphenyl and derivative molecules by using the B3LYP functional and the 3-21G basis set, as well as the optimization structure. The calculated values of HOMO and LUMO energies, as well as predicted by ChemBioDraw program ^{1}H and ^{13}C NMR spectra for the studied compounds are in a good agreement with experimental data. All properties were calculated by using Gaussian 09 program and GaussianView 5.08 program, except NMR characteristics.

Keywords: DFT calculation, electronic properties, IR and NMR spectra, biphenyl molecule.

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